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EXISTENCE OF SOLUTIONS TO SYSTEMS OF UNDERDETERMINED EQUATIONS AND SPHERICAL DESIGNS*

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Abstract. This paper is concerned with proving the existence of solutions to an underdetermined system of equations and with the application to existence of spherical t-designs with $(t+1)^2$ points on the unit sphere S^2 in R^3. We show that the construction of spherical designs is equivalent to solution of underdetermined equations. A new verification method for underdetermined equations is derived using Brouwer's fixed point theorem. Application of the method provides spherical t-designs which are close to extremal (maximum determinant) points and have the optimal order $O(t^2)$ for the number of points. An error bound for the computed spherical designs is provided.

Key words. verification, underdetermined system, spherical designs, extremal points, interpolation, numerical integration

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1. Introduction.

Let $c : R^n \to R^m$ be a continuously differentiable function with $m < n$. Suppose that $\hat{x}$ is an approximate solution of the underdetermined system of nonlinear equations

$$c(x) = 0 \tag{1.1}$$

and the Jacobian $c'(x)$ of c at $\hat{x}$ has full row rank. We are interested in the existence of a solution of (1.1) in a neighborhood of $\hat{x}$.

Underdetermined systems of equations arise in constrained optimization problems, continuation methods for underdetermined equations, etc. [3, 12, 14, 21]. This paper gives a verification method for solutions of the underdetermined equations (1.1). The main difficulty in proving the existence of solutions of an underdetermined system of equations is that the Jacobian $c'(x)$ is an $m \times n$ matrix with $m < n$. Let $c'(\hat{x})^+$ be the Moore–Penrose pseudoinverse of $c'(\hat{x})$. A popular method for verifying the existence of solutions of nonlinear equations is to use a Krawczyk-type interval operator [1]. Replacing the inverse by a Moore–Penrose pseudoinverse, we can get a Krawczyk-type interval operator

$$\mathcal{K}(X) = \hat{x} - c'(\hat{x})^+ c(\hat{x}) + (I - c'(\hat{x})^+ C'(X))(X - \hat{x}), \tag{1.2}$$

where X is an interval in R^n defined by

$$X = [\hat{x} - h, \hat{x} + h], \qquad h \in R^n, \quad h \geq 0,$$

and $C'(X)$ is an interval arithmetic evaluation satisfying

$$c'(x) \in C'(X) \qquad \text{for } x \in X.$$

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It can be shown [1] that there is a solution of (1.1) in X if

$$\mathcal{K}(X) \subseteq X \tag{1.3}$$

and $c'(\hat{x})$ has full row rank. However, the enclosure (1.3) rarely holds due to the equality [8]

$$\|I - c'(\hat{x})^+ c'(\hat{x})\|_2 = \min\{1, n - m\}$$

and the fact that

$$\mathcal{K}(X) \subseteq X \quad \Rightarrow \quad \|I - c'(\hat{x})^+ c'(x)\|_\infty \leq 1 \quad \forall\, x \in X.$$

In section 2 we present a new verification method for underdetermined systems of (1.1) which does not need the generalized inverse $c'(\hat{x})^+$.

A cubature (numerical integration) rule for the unit sphere $S^2 = \{y \in R^3 : \|y\|_2 = 1\}$ is a set of N points $y_\ell \in S^2$ and weights w_ℓ for $\ell = 1, \ldots, N$ such that

$$\int_{S^2} f(y)dy \approx \sum_{\ell=1}^{N} w_\ell f(y_\ell).$$

Let $\mathbb{P}_t \equiv \mathbb{P}_t(S^2)$ be the linear space of restrictions of polynomials of degree $\leq t$ in 3 variables to S^2. The dimension of the space $\mathbb{P}_t$ is $d_t := (t+1)^2$. Spherical t-designs, introduced in [5], are sets of N points $\{y_1, y_2, \ldots, y_N\} \subset S^2$ such that the equally weighted ($w_\ell = |S^2|/N = 4\pi/N$, $\ell = 1, \ldots, N$) cubature rule is exact for all spherical polynomials of degree at most t, that is,

$$\int_{S^2} p(y)dy = \frac{4\pi}{N} \sum_{\ell=1}^{N} p(y_\ell) \qquad \forall p \in \mathbb{P}_t.$$

For $t \geq 1$, the existence of a spherical t-design was proved in [19]. Commonly, the interest is in the smallest number N_t^* of points required to give a spherical t-design. Lower bounds on N_t^* given in [5] are

$$\begin{aligned} N_t^* &\geq \frac{(t+1)(t+3)}{4} && \text{if } t \text{ is odd,} \\ N_t^* &\geq \frac{(t+2)^2}{4} && \text{if } t \text{ is even.} \end{aligned}$$

A spherical t-design which achieves the lower bounds is called a tight spherical t-design. However, for $t \geq 2$, it is known that tight spherical t-designs do not exist [5]. Hardin and Sloane [7] have extensively investigated spherical designs on S^2 and suggested a sequence of putative spherical t-designs with $\frac{1}{2}t^2 + o(t^2)$ points. A 7-design with 24 points was first found by McLaren in 1963 [13]. Korevaar and Meyers [10] considered the construction for spherical t-designs with $O(t^3)$ points on S^2. An approach for the numerical calculation of spherical designs using multiobjective optimization was studied by Maier [11], and computational proof of the existence of spherical designs using interval methods [9] was investigated by Hardin and Sloane [7].

Extremal (or maximum determinant) points [20] are sets of $(t+1)^2$ points on S^2 which maximize the determinant of a basis matrix for an arbitrary basis of $\mathbb{P}_t$. Sloan and Womersley [20, 22] showed that extremal systems have very nice geometrical properties as the points are well separated and the computed interpolatory cubature weights are positive ($w_\ell > |S^2|/(2N)$ for $\ell = 1, \ldots, N$ for degrees up to $t = 150$). Also the condition number of the basis matrix grows slowly, giving confidence in the calculated cubature weights. Proving the positivity of the cubature weights for all degrees t for the extremal points is still an open question. Other systems of points, such as minimum energy points, often have basis matrices with such high condition numbers that no confidence can be placed in the calculated cubature weights.

Equal weight cubature rules, or spherical designs, are simpler to implement and there is no question about the positivity of the weights. There are many different characterizations of spherical t-designs [6]. However, these can be very ill conditioned. Extremal points provide excellent starting points for numerically finding solutions to an underdetermined, but highly nonlinear, system of equations which characterize spherical t-designs with $(t+1)^2$ points. Application of the verification method to the system of equations then proves the existence of spherical t-designs which are close to the calculated points and have the optimal order $O(t^2)$ for the number of points. Moreover, spherical designs with $(t+1)^2$ points which also have a basis matrix with a determinant close to the maximum are simultaneously good for cubature and interpolation. Computed spherical t-designs with $(t+1)^2$ points for degrees up to $t = 50$ are available from http://www.maths.unsw.edu.au/∼rsw/Sphere.

The focus here is not on finding a spherical t-design with the minimal number of points, but rather proving the existence of spherical t-designs with $(t+1)^2$ points close to an extremal system. Once existence of a spherical design with $(t+1)^2$ points is established one can then look for *extremal spherical designs*, that is, systems of $(t+1)^2$ points which maximize the determinant of a basis matrix subject to the constraints that they are spherical t-designs.

In section 3 we reformulate the calculation of a spherical t-design with $(t+1)^2$ points as an underdetermined system of nonlinear equations (1.1) with $m = (t+1)^2-1$ equations and $n = 2(t+1)^2 - 3$ variables. We show that a sufficient and necessary condition for the existence of solutions to the system of equations is existence of a spherical t-design with $(t+1)^2$ points. In section 4, we apply the verification method to find new spherical t-designs. The computed spherical designs $\hat{Y} = \{\hat{y}_1, \ldots, \hat{y}_{d_t}\}$ are compared with the extremal (maximum determinant) points, and error bounds of $\hat{Y}$ to exact spherical designs are given.

For a given $m \times n$ matrix A, let $A_{\mathcal{I}}$ be the submatrix of A whose entries lie in the columns of A indexed by $\mathcal{I}$. For a given vector $x \in R^n$, let $x_{\mathcal{I}}$ be the subvector of x whose entries of x are indexed by $\mathcal{I}$.

2. A verification method. Let $\hat{x}$ be a computed solution of (1.1). Let $\mathcal{B}$ be an index set $\{k_1, k_2, \ldots, k_m\}$ such that $c'_{\mathcal{B}}(\hat{x}) \in R^{m\times m}$ is nonsingular. Define the function $H : R^n \to R^n$ by

$$H_{\mathcal{B}}(x) = x_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}c(x), \tag{2.1}$$

$$H_{\mathcal{N}}(x) = x_{\mathcal{N}} - \alpha(x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}), \tag{2.2}$$

where $\mathcal{N} = \{1, 2, \ldots, n\}/\mathcal{B}$ and $\alpha \in (0, 1)$ is a constant. Obviously, if $x^* \in R^n$ is a fixed point of H, that is, $H(x^*) = x^*$, then we have $c(x^*) = 0$ with $x^*_{\mathcal{N}} = \hat{x}_{\mathcal{N}}$. Choose two nonnegative numbers r_1 and r_2 and define the convex set

$$X = \{\, x \in R^n : \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \le r_1, \|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\| \le r_2 \}\,.$$

THEOREM 2.1. *Suppose that* $c : R^n \to R^m$ *is continuously differentiable,* c' *has full row rank at* $\hat{x}$*, and*

$$\|c'_{\mathcal{B}}(x) - c'_{\mathcal{B}}(\hat{x})\| \le K\|x - \hat{x}\| \text{ for } x \in X. \tag{2.3}$$

(1) *There is a solution of* (1.1) *in* X *if*

$$\|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\frac{1}{2}K(r_1 + r_2)r_1 + \max_{x\in X}\|c'_{\mathcal{N}}(x)\|r_2\right) \le r_1. \tag{2.4}$$

(2) *There is no solution of* (1.1) *in* X *if*

$$\|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| - \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\frac{1}{2}K(r_1 + r_2)r_1 + \max_{x\in X}\|c'_{\mathcal{N}}(x)\|r_2\right) > r_1. \tag{2.5}$$

Proof. (1) By the continuity of $c'(x)$ and the mean value theorem, we find

$$\begin{aligned}
H_{\mathcal{B}}(x) &= \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x}) + x_{\mathcal{B}} - \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}(c(x) - c(\hat{x}))\\
&= \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x}) + x_{\mathcal{B}} - \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}\int_0^1 c'(x + t(\hat{x} - x))(x - \hat{x})dt\\
&= \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x}) + x_{\mathcal{B}} - \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}\int_0^1 c'_{\mathcal{B}}(x + t(\hat{x} - x))(x_{\mathcal{B}} - \hat{x}_{\mathcal{B}})dt\\
&\quad -c'_{\mathcal{B}}(\hat{x})^{-1}\int_0^1 c'_{\mathcal{N}}(x + t(\hat{x} - x))(x_{\mathcal{N}} - \hat{x}_{\mathcal{N}})dt\\
&= \hat{x}_{\mathcal{B}} - c'_{\mathcal{B}}(\hat{x})^{-1}\left[c(\hat{x}) + \int_0^1 (c'_{\mathcal{B}}(\hat{x}) - c'_{\mathcal{B}}(x + t(\hat{x} - x)))(x_{\mathcal{B}} - \hat{x}_{\mathcal{B}})dt\right.\\
&\qquad\left. + \int_0^1 c'_{\mathcal{N}}(x + t(\hat{x} - x))(x_{\mathcal{N}} - \hat{x}_{\mathcal{N}})dt\right].
\end{aligned}$$

Therefore, for any $x \in X$, we have

$$\begin{aligned}
&\|H_{\mathcal{B}}(x) - \hat{x}_{\mathcal{B}}\|\\
&\le \|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \int_0^1 \|c'_{\mathcal{B}}(\hat{x}) - c'_{\mathcal{B}}(x + t(\hat{x} - x))\|\|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\|dt\\
&\quad + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \int_0^1 \|c'_{\mathcal{N}}(x + t(\hat{x} - x))\|\|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\|dt\\
&\le \|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\int_0^1 (1-t)K\|\hat{x} - x\|r_1 dt + \int_0^1 \max_{x\in X}\|c'_{\mathcal{N}}(x)\|r_2 dt\right)\\
&\le \|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\frac{1}{2}K(r_1 + r_2)r_1 + \max_{x\in X}\|c'_{\mathcal{N}}(x)\|r_2\right).
\end{aligned}$$

Here we use the facts that $x + t(\hat{x} - x) \in X$, $\|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \le r_1$, and $\|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\| \le r_2$ for all $x \in X$ and $t \in [0, 1]$.

This implies that if (2.4) holds, then for any $x \in X$ we have

$$\|H_{\mathcal{B}}(x) - \hat{x}_{\mathcal{B}}\| \le r_1.$$

Moreover, by the definition of H, we always have

$$\|H_{\mathcal{N}}(x) - \hat{x}_{\mathcal{N}}\| = (1 - \alpha)\|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\| \le r_2.$$

Therefore, (2.4) implies that H maps X into itself; that is,

$$H(x) \in X \quad \text{for any } x \in X. \tag{2.6}$$

Using Brouwer's fixed point theorem, (2.6) implies that there is a fixed point x^* of H in X. From the definition of H, x^* is a solution of (1.1).

(2) Assume that (2.5) holds and there is a solution x^* in X. Following the proof for part (1), we have

$$\begin{aligned} r_1 &\geq \|x^*_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \\ &= \|H_{\mathcal{B}}(x^*) - \hat{x}_{\mathcal{B}}\| \\ &\geq \|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| - \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \int_0^1 \|c'_{\mathcal{B}}(\hat{x}) - c'_{\mathcal{B}}(x^* + t(\hat{x} - x^*))\| \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| dt \\ &\quad - \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \int_0^1 \|c'_{\mathcal{N}}(x^* + t(\hat{x} - x^*))\| \|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\| dt \\ &\geq \|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| - \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\frac{1}{2} K(r_1 + r_2)r_1 + \max_{x \in X} \|c'_{\mathcal{N}}(x)\| r_2 \right) > r_1. \end{aligned}$$

This is a contradiction, which completes the proof. □

Without loss of generality, we assume that $r_1 \neq 0$. Let $\tau \in (0, \frac{1}{2})$. Define a subset of X:

$$X_\tau = \{\, x \mid \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \leq \tau r_1, \|x_{\mathcal{N}} - \hat{x}_{\mathcal{N}}\| \leq \tau r_2\}.$$

Then we have the following corollary.

Corollary 2.2. *Under the assumptions of Theorem* 2.1*, inequality* (2.4) *implies that $c'_{\mathcal{B}}(x)$ is nonsingular for all $x \in X_\tau$ and the solution x^* of* (1.1) *with $x^*_{\mathcal{N}} = \hat{x}_{\mathcal{N}}$ is unique in X_τ.*

Proof. For any $x \in X_\tau$ $(x \neq \hat{x})$, inequality (2.4) implies that

$$\begin{aligned} r_1 &\geq \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \frac{1}{2} K(r_1 + r_2) r_1 \\ &\geq \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \frac{1}{2\tau} K \|x - \hat{x}\| r_1 \\ &> \|c'_{\mathcal{B}}(\hat{x})^{-1}\| K \|x - \hat{x}\| r_1 \\ &\geq r_1 \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \|c'_{\mathcal{B}}(\hat{x}) - c'_{\mathcal{B}}(x)\| \\ &\geq r_1 \|I - c'_{\mathcal{B}}(\hat{x})^{-1} c'_{\mathcal{B}}(x)\|. \end{aligned}$$

Dividing r_1 in both sides, we find

$$\|I - c'_{\mathcal{B}}(\hat{x})^{-1} c'_{\mathcal{B}}(x)\| < 1.$$

Hence $c'_{\mathcal{B}}(x)$ is nonsingular. By the implicit function theorem [16], the solution x^* of (1.1) with $x^*_{\mathcal{N}} = \hat{x}_{\mathcal{N}}$ is unique in X_τ. □

Remark 2.1. For the case $m = n$, we have $x = x_{\mathcal{B}}$, $c'_{\mathcal{B}}(x) = c'(x)$, and (2.4) reduces to

$$\|c'(\hat{x})^{-1}c(\hat{x})\| + \frac{1}{2} K \|c'(\hat{x})^{-1}\| r^2 \leq r. \tag{2.7}$$

This is a quadratic inequality in r. If

$$\rho := K\|c'(\hat{x})^{-1}c(\hat{x})\|\|c'(\hat{x})^{-1}\| \leq \frac{1}{2}, \tag{2.8}$$

then (2.7) holds for all r satisfying

$$\frac{1-\sqrt{1-2\rho}}{K\|c'(\hat{x})^{-1}\|} \leq r \leq \frac{1+\sqrt{1-2\rho}}{K\|c'(\hat{x})^{-1}\|}.$$

By Theorem 2.1, there is a solution in $X = \{x \in R^n : \|x - \hat{x}\| \leq r\}$. Therefore, Theorem 2.1 is a generalization of the Kantorovich theorem [16] for the existence of the solution.

3. Spherical designs. In this section we describe a method of reformulating construction of spherical t-designs as an underdetermined system of nonlinear equations.

For a given positive integer t, a set of points $Y = \{y_1, \ldots, y_{d_t}\} \subset S^2$ is called a fundamental system if the zero polynomial is the only member of $\mathbb{P}_t$ that vanishes at each point y_j, $j = 1, 2, \ldots, d_t$. The requirement

$$d_t = (t+1)^2 = \dim \mathbb{P}_t$$

ensures that the basis matrix is square.

Y is called an extremal system if these points maximize the determinant of the interpolation matrix with respect to an arbitrary basis of $\mathbb{P}_t$. An extremal system is obviously a fundamental system. Sloan and Womersley [20] showed that the extremal fundamental systems have excellent geometrical properties and surprisingly good performance for numerical integration. However, it is unknown whether there is always a spherical t-design in a neighborhood of an extremal fundamental system. Our aim is to verify its existence.

Let $L_\ell : [-1, 1] \to R$ be the usual Legendre polynomial [2]. The Rodrigues representation yields

$$L_\ell(z) = \frac{1}{2^\ell} \sum_{k=0}^{[\ell/2]} \frac{(-1)^k (2\ell - 2k)!}{k!(\ell - k)!(\ell - 2k)!} z^{\ell - 2k}, \tag{3.1}$$

where $[\ell/2]$ is the floor function. Let

$$J_t(z) = \frac{1}{4\pi} \sum_{\ell=0}^{t} (2\ell + 1) L_\ell(z), \qquad z \in [-1, 1],$$

which is a normalized Jacobi polynomial. The Gram matrix $G \equiv G(Y)$ is a symmetric positive semidefinite $d_t \times d_t$ matrix with elements

$$G_{i,j} = J_t(y_i^T y_j).$$

The functions

$$g_i(y) = J_t(y_i^T y), \ i = 1, \ldots, d_t, \ y \in S^2,$$

belong to $\mathbb{P}_t$. If G is nonsingular, $\{g_1, \ldots, g_{d_t}\}$ is a basis for $\mathbb{P}_t$. For a given arbitrary function $f \in C(S^2)$, the unique polynomial interpolant Λf for the set Y is

$$(\Lambda f)(y) = \sum_{i=1}^{d_t} v_i g_i(y).$$

Here the vector of weights $v = (v_1, \ldots, v_{d_t})$ is the solution of the linear system of equations

$$Gv = b, \tag{3.2}$$

where $b_i = f(y_i), i = 1, 2 \ldots, d_t$.

The cubature rule

$$Q_{d_t}(f) = \sum_{i=1}^{d_t} w_i f(y_i) \approx \int_{S^2} f(y) dy$$

is exact for all polynomials p of degree $\leq t$ if w satisfies the system of linear equations

$$Gw = e, \tag{3.3}$$

where $e = (1, 1, \ldots, 1)^T \in R^{d_t}$. In particular, the cubature rule is exact for the constant polynomial $1 \in \mathbb{P}_t$. Thus

$$\int_{S^2} 1 \; dy = |S^2| = 4\pi = \sum_{i=1}^{d_t} w_i.$$

Hence the average cubature weight is

$$w_{\text{avg}} = \frac{4\pi}{d_t}.$$

Numerical results given in [22] show that the weights defined by (3.3) with the coefficient matrix $G(\bar{Y})$, where

$$\log \det G(\bar{Y}) = \max_{Y \subset S^2} \; \log \det G(Y), \tag{3.4}$$

are all positive and the scaled weights w_i / w_{avg} lie in $[1/2, 3/2]$.

The set of points $\bar{Y} = \{\bar{y}_1, \ldots, \bar{y}_{d_t}\}$ defined by (3.4) is an extremal fundamental system. It is conjectured that there is a spherical t-design which is very close to an extremal fundamental system; that is, there is a set of points $Y^* = \{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ in a neighborhood of $\bar{Y} = \{\bar{y}_1, \ldots, \bar{y}_{d_t}\}$ such that

$$\int_{S^2} p(y) dy = \sum_{i=1}^{d_t} w_i p(y_i^*) \qquad \forall p \in \mathbb{P}_t$$

and equal weights

$$w_i = \frac{4\pi}{d_t}, \;\; i = 1, 2, \ldots, d_t. \tag{3.5}$$

To explore this conjecture, we reformulate the problem as an underdetermined system of nonlinear equations. The matrix G is rotationally invariant, so the set of points can be normalized so that the first point is at the north pole and the second is on the prime meridian. Hence a spherical parametrization $\theta_j \in [0, \pi]$ and $\phi_j \in [0, 2\pi)$ of the points y_j, $j = 1, 2, \ldots, d_t$, has $\phi_1 = 0$, $\theta_1 = 0$, and $\phi_2 = 0$, giving a total of $2d_t - 3$ variables.

Let

$$n = 2d_t - 3, \qquad m = d_t - 1,$$

and let

$$\begin{aligned} x_{i-1} &= \theta_i, & i &= 2, 3, \ldots, d_t, \\ x_{d_t+i-3} &= \phi_i, & i &= 3, 4, \ldots, d_t. \end{aligned}$$

The set of points $Y = \{y_1, \ldots, y_{d_t}\}$ and the vector of variables $x \in R^n$ are uniquely related by

$$y_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad y_2 = \begin{bmatrix} \sin x_1 \\ 0 \\ \cos x_1 \end{bmatrix}, \quad y_i = \begin{bmatrix} \sin\theta_i \cos\phi_i \\ \sin\theta_i \sin\phi_i \\ \cos\theta_i \end{bmatrix} = \begin{bmatrix} \sin x_{i-1} \cos x_{d_t+i-3} \\ \sin x_{i-1} \sin x_{d_t+i-3} \\ \cos x_{i-1} \end{bmatrix}.$$

The simple bounds on θ_i and ϕ_i can be ignored due to the periodicity of the sin and cos functions. Hence the matrix G can be regarded as a function of x whose elements are defined by

$$G_{i,j}(x) = J_t(y_i^T y_j).$$

Define the function $c : R^n \to R^m$ by

$$c(x) = EG(x)e, \tag{3.6}$$

where E is the $m \times d_t$ matrix

$$E = \begin{pmatrix} 1 & -1 & 0 & \ldots & 0 \\ 1 & 0 & -1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 1 & 0 & \ldots & 0 & -1 \end{pmatrix}.$$

This is motivated by the simple, but critical, observation that any cubature rule which is exact for constants has $\sum_{i=1}^{d_t} w_i = 4\pi$, so one only requires that $w_1 = w_i$ for $i = 2, \ldots, d_t$ to get (3.5). In fact the system of d_t equations $G(x)e - w_{avg}e = 0$ has a Jacobian with only rank $d_t - 1$.

The following theorem states the relation between a spherical t-design and a zero of the function c defined by (3.6).

THEOREM 3.1. *Suppose that $G(x^*)$ is nonsingular. Then x^* corresponds to a spherical t-design with $(t+1)^2$ points if and only if $c(x^*) = 0$.*

Proof. Let x^* be a solution of $c(x) = 0$, and let $\{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ be the set of points defined by x^*. First it is shown that $\{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ is a spherical t-design.

Since $G(x^*)$ is nonsingular, $\{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ is a fundamental system and the functions

$$g_j(y) = G(y_j^{*T} y), \quad j = 1, 2, \ldots, d_t,$$

form a basis of $\mathbb{P}_t$. Hence for any $p \in \mathbb{P}_t$ there are scalars $\alpha_j, j = 1, \ldots, d_t$, such that

$$p(y) = \sum_{j=1}^{d_t} \alpha_j g_j(y).$$

Note that (see [17] for an example)

$$\int_{S^2} g_j(y)dy = 1 \quad \forall\, j = 1, \ldots, d_t. \tag{3.7}$$

Moreover, $c(x^*) = 0$ implies that all components of $G(x^*)e$ are equal. Hence we can write

$$G(x^*)e = \mu e,$$

where μ is a scalar. Because of the nonsingularity of $G(x^*)$, $\mu \neq 0$. This yields

$$\int_{S^2} g_j(y)dy = 1 = \frac{1}{\mu} \sum_{k=1}^{d_t} G_{j,k}(x^*), \qquad j = 1, 2, \ldots, d_t.$$

We calculate the integral

$$\begin{aligned}
\int_{S^2} p(y)dy &= \sum_{j=1}^{d_t} \alpha_j \int_{S^2} g_j(y)dy \\
&= \frac{1}{\mu} \sum_{j=1}^{d_t} \alpha_j \sum_{k=1}^{d_t} G_{j,k}(x^*) \\
&= \frac{1}{\mu} \sum_{k=1}^{d_t} \sum_{j=1}^{d_t} \alpha_j G_{j,k}(x^*) \\
&= \frac{1}{\mu} \sum_{k=1}^{d_t} \sum_{j=1}^{d_t} \alpha_j g_j(y_k^*) \\
&= \frac{1}{\mu} \sum_{k=1}^{d_t} p(y_k^*).
\end{aligned}$$

In particular, for $p(y) \equiv 1$, the area of the sphere is

$$|S^2| = 4\pi = \int_{S^2} p(y)dy = \frac{1}{\mu} \sum_{k=1}^{d_t} p(y_k^*) = \frac{d_t}{\mu}.$$

Thus $\mu = d_t/4\pi$, and therefore $\{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ is a spherical t-design.

Now we prove that $c(x^*) = 0$ if x^* corresponds to a spherical t-design with $(t+1)^2$ points. By the definition of a spherical t-design, for any $p \in \mathbb{P}_t$,

$$\int_{S^2} p(y)dy = \frac{4\pi}{d_t} \sum_{k=1}^{d_t} p(y_k^*).$$

In particular, as $g_j \in \mathbb{P}_t$,

$$\int_{S^2} g_j(y)dy = \frac{4\pi}{d_t}\sum_{k=1}^{d_t} g_j(y_k^*), \qquad j = 1, 2, \dots, d_t.$$

Hence, from the definition of g_j and (3.7), we find

$$\frac{4\pi}{d_t}\sum_{k=1}^{d_t} G_{j,k}(x^*) = \frac{4\pi}{d_t}\sum_{k=1}^{d_t} g_j(y_k^*) = 1.$$

This implies

$$G(x^*)e = \frac{d_t}{4\pi}e,$$

and thus

$$c(x^*) = EG(x^*)e = \frac{d_t}{4\pi}Ee = 0. \qquad \square$$

Let $\hat{x} \in R^n$ correspond to the set of points $\hat{Y} = \{\hat{y}_1, \dots, \hat{y}_{d_t}\}$ on the sphere. The condition for the cubature rule

$$Q_{d_t}(f) = \sum_{i=1}^{d_t} w_i f(\hat{y}_i)$$

to be exact for all polynomials in $\mathbb{P}_t$ is that $w = (w_1, \dots, w_{d_t})^T$ is the solution of

$$G(\hat{x})w = e.$$

From Theorem 3.1, we know that $w = G(\hat{x})^{-1}e = (4\pi/d_t)e$ if and only if $c(\hat{x}) = 0$. The following theorem gives a result of the weights for the case $c(\hat{x}) \neq 0$.

THEOREM 3.2. *Suppose that $G(\hat{x})$ is nonsingular. Let $w = G(\hat{x})^{-1}e$. Then*

$$\max_{1\le i\le d_t} |w_1 - w_i| \le \frac{4}{\|G(\hat{x})e\|_\infty}\|G(\hat{x})^{-1}\|_\infty \|c(\hat{x})\|_\infty. \tag{3.8}$$

Proof. Let $\|\cdot\| = \|\cdot\|_\infty$ and let $|(G(\hat{x})e)_{i_0}| = \|G(\hat{x})e\|$. Then $\mu := (G(\hat{x})e)_{i_0} \neq 0$ and

$$\begin{aligned}\|\mu e - G(\hat{x})e\| &\le \|\mu e - (G(\hat{x})e)_1 e\| + \|(G(\hat{x})e)_1 e - G(\hat{x})e\| \\ &\le 2\|c(\hat{x})\|.\end{aligned}$$

Now, by the definition of the matrix E, we have

$$\begin{aligned}\max_{1\le i\le d_t} |w_1 - w_i| &= \|EG(\hat{x})^{-1}e\| \\ &= \|EG(\hat{x})^{-1}e - \frac{1}{\mu}Ee\| \\ &= \frac{1}{|\mu|}\|\mu EG(\hat{x})^{-1}e - EG(\hat{x})^{-1}G(\hat{x})e\| \\ &= \frac{1}{|\mu|}\|EG(\hat{x})^{-1}(\mu e - G(\hat{x})e)\| \\ &\le \frac{2}{|\mu|}\|E\|\|G(\hat{x})^{-1}\|\|c(\hat{x})\| \\ &= \frac{4}{|\mu|}\|G(\hat{x})^{-1}\|\|c(\hat{x})\|. \qquad \square\end{aligned}$$

4. Numerical verification of spherical t-designs. In this section, we use Theorems 2.1 and 3.1 to verify the existence of spherical t-designs. In particular, we use (2.4) to verify the existence of solutions to the system

$$c(x) := EG(x)e = 0. \tag{4.1}$$

Note that the highly nonlinear function $c(\cdot)$ is in $C^\infty(R^n)$ as long as the points are not at the south pole, which can easily be checked. (The first point is always the north pole and is not allowed to vary.) To save computational cost, let $x_\mathcal{B} = (x_1, \dots, x_{d_t-1})^T$ and set $r_2 = 0$. Hence $c'_\mathcal{B}(x)$ is the first $(d_t - 1)$ columns of $c'(x)$ for $x \in X$, where

$$X = \{x \mid \|x_\mathcal{B} - \hat{x}_\mathcal{B}\| \le r_1,\ x_\mathcal{N} = \hat{x}_\mathcal{N}\}.$$

The expansion (3.1) is used to calculate the derivatives of $c_i(x)$. Moreover, we can give an upper bound for the second derivatives. Since for $i, j = 1, \dots, d_t$, $G_{ij}(x)$ are polynomials of degree t, the function

$$c_i(x) = (G(x)e)_1 - (G(x)e)_{i+1} = \frac{1}{4\pi}\sum_{j=1}^{d_t}\sum_{\ell=0}^{t}(2\ell+1)\left(L_\ell(y_1^T y_j) - L_\ell(y_{i+1}^T y_j)\right)$$

is polynomial of degree $\le t$. The first derivative of c_i is

$$\frac{\partial c_i(x)}{\partial x_k} = \frac{1}{4\pi}\sum_{j=1}^{d_t}\sum_{\ell=0}^{t}(2\ell+1)\left(L'_\ell(y_1^T y_j)\frac{\partial(y_1^T y_j)}{\partial x_k} - L'_\ell(y_{i+1}^T y_j)\frac{\partial(y_{i+1}^T y_j)}{\partial x_k}\right),$$

and the second derivative of c_i is

$$\frac{\partial^2 c_i(x)}{\partial x_k \partial x_\nu} = \frac{1}{4\pi}\sum_{j=1}^{d_t}\sum_{\ell=0}^{t}(2\ell+1)\Bigg(L''_\ell(y_1^T y_j)\frac{\partial(y_1^T y_j)}{\partial x_k}\frac{\partial(y_1^T y_j)}{\partial x_\nu} + L'_\ell(y_1^T y_j)\frac{\partial^2(y_1^T y_j)}{\partial x_k \partial x_\nu}$$

$$-L''_\ell(y_{i+1}^T y_j)\frac{\partial(y_{i+1}^T y_j)}{\partial x_k}\frac{\partial(y_{i+1}^T y_j)}{\partial x_\nu} - L'_\ell(y_{i+1}^T y_j)\frac{\partial^2(y_{i+1}^T y_j)}{\partial x_k \partial x_\nu}\Bigg).$$

Note that we consider only the first $(d_t - 1)$ columns of $c'(x)$ with respect to $x_\mathcal{B}$. Let

$$\nabla y_2 = \begin{bmatrix} \cos x_1 \\ 0 \\ -\sin x_1 \end{bmatrix}, \qquad \nabla y_i = \begin{bmatrix} \cos x_{i-1}\cos x_{d_t+i-3} \\ \cos x_{i-1}\sin x_{d_t+i-3} \\ -\sin x_{i-1} \end{bmatrix}.$$

For $k, \nu \le d_t - 1$, we have

$$\frac{\partial(y_1^T y_j)}{\partial x_k} = \begin{cases} y_1^T \nabla y_j & \text{if } k = j-1, \\ 0 & \text{otherwise;} \end{cases} \qquad \frac{\partial^2(y_1^T y_j)}{\partial x_k \partial x_\nu} = \begin{cases} -y_1^T y_j & \text{if } k = \nu = j-1, \\ 0 & \text{otherwise;} \end{cases}$$

$$\frac{\partial(y_{i+1}^T y_j)}{\partial x_k} = \begin{cases} y_{i+1}^T \nabla y_j & \text{if } k = j-1, \\ y_j^T \nabla y_{i+1} & \text{if } k = i, \\ 0 & \text{otherwise;} \end{cases} \qquad \frac{\partial^2(y_{i+1}^T y_j)}{\partial x_k \partial x_\nu} = \begin{cases} -y_{i+1}^T y_j & \text{if } k = \nu = j-1 \\ & \text{or } k = \nu = i, \\ \nabla y_i^T \nabla y_j & \text{if } k = j-1, \nu = i \\ & \text{or } k = i, \nu = j-1, \\ 0 & \text{otherwise.} \end{cases}$$

We use the relations $|y_i^T y_j| \leq 1$ and $|\nabla y_i^T y_j| \leq 1$ to give an upper bound K for the second derivatives of $c(\cdot)$ with respect to the first $d_t - 1$ variables. This, together with $x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}$, implies

$$\|c'_{\mathcal{B}}(x) - c'_{\mathcal{B}}(\hat{x})\| \leq K\|x - \hat{x}\|.$$

The infinity norm was used in the numerical implementation, so in the rest of this section $\|\cdot\|$ denotes $\|\cdot\|_\infty$.

The procedure for verifying the existence of a spherical t-designs is as follows:

1. Find an approximate solution $\hat{x}$ of $c(x) = 0$ starting from $\bar{x}$ corresponding to an extremal fundamental system $\bar{Y}$.
2. Calculate $c'_{\mathcal{B}}(\hat{x})$ and K.
3. Calculate

$$\rho = K\|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| \, \|c'_{\mathcal{B}}(\hat{x})^{-1}\|. \tag{4.2}$$

If $\rho \leq \frac{1}{2}$, then there is a solution of (4.1) in the set

$$X = \{x \in R^n : \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \leq r_1, x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\},$$

where

$$r_1 = \frac{1 - \sqrt{1 - 2\rho}}{K\|c'_{\mathcal{B}}(\hat{x})^{-1}\|}.$$

If $\rho > \frac{1}{2}$, then (4.1) has no solution in

$$X = \{x \in R^n : \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \leq \gamma_1, x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\},$$

where

$$\gamma_1 = \frac{\sqrt{1 + 2\rho} - 1}{K\|c'_{\mathcal{B}}(\hat{x})^{-1}\|}.$$

Note that the natural residual $\|c(x)\|_2$ has many local minimizers. To find a good approximate solution of $c(x) = 0$, we choose several starting points around the extremal system and use the Gauss–Newton method with line search. The interest in starting from an extremal system stems from Figure 2 in [20] and Theorem 3.1. The cubature weights for the computed extremal system of [20] are very close to $4\pi/d_t$ and they maximize the determinant $G(x)$. Extremal systems can be downloaded from http://www.maths.unsw.edu.au/∼rsw/Sphere.

Numerical results are given in Table 1, where $\bar{x}$ is the vector corresponding to an extremal fundamental system $\bar{Y}$, $\hat{x}$ is an approximate solution of $c(x) = 0$,

$$\hat{w} = G(\hat{x})^{-1}e$$

is the weight for the cubature rule, and $\hat{Y} = \{\hat{y}_1, \ldots, \hat{y}_{d_t}\}$ is the set of points corresponding to $\hat{x}$.

As the cubature rule is exact for the constant polynomial $1 \in \mathbb{P}_t$, the average weight is $\hat{w}_{avg} = 4\pi/d_t$. From the last column of Table 1, we see that all weights are positive and

$$\left|\hat{w}_i - \frac{4\pi}{d_t}\right| \leq w_{\max} - w_{\min} \approx 0.$$

TABLE 1

Extremal points $\bar{x}$, computed spherical designs $\hat{x}$, exact spherical design x^*, $\|\hat{x} - x^*\| \le r_1$, $x \in R^{2(t+1)^2-3}$.

t	d_t	$\|c(\bar{x})\|$	$\|c(\hat{x})\|$	log det$G(\bar{x})$	log det$G(\hat{x})$	r_1	$\|\bar{x} - \hat{x}\|$	$\hat{w}_{\max} - \hat{w}_{\min}$
2	9	0.0245	4.44e-16	-3.2134	-3.2157	1.01e-15	0.0255	1.55e-15
3	16	0.4299	2.66e-15	3.3867	2.5779	2.36e-15	0.2742	1.88e-15
4	25	0.3898	7.32e-15	16.1396	15.9337	1.80e-14	0.1002	3.33e-15
5	36	0.6318	7.54e-15	36.1736	35.4829	1.34e-14	0.2595	2.10e-14
6	49	1.1376	2.62e-14	64.0948	62.6443	3.45e-14	0.1918	3.88e-15
7	64	0.9189	6.03e-14	100.6942	100.4167	5.07e-14	0.1277	4.10e-15
8	81	1.3713	1.92e-13	146.1926	144.3611	1.15e-13	0.2974	8.54e-15
9	100	1.4023	4.52e-13	201.5589	186.2265	1.84e-13	0.2526	7.88e-13
10	121	3.7879	8.07e-13	266.3178	265.5019	6.14e-11	0.0358	2.40e-14

Hence the set $\hat{Y}$ can be considered as computed spherical t-designs. These designs are new. Moreover, from Theorem 2.1 and $\|\hat{x} - x^*\| \le r_1$, an error bound for the computed spherical t-designs to an exact spherical design $\{y_1^*, \dots, y_{d_t}^*\}$ corresponding to the exact solution x^* of $c(x) = 0$ is

$$\max_{1 \le i \le d_t} \|y_i^* - \hat{y}_i\| \le 2\|\hat{x} - x^*\| \le 2r_1,$$

where the first inequality uses the relation between x and y.

The numerical results also give an error bound for the extremal system

$$\begin{aligned} \max_{1 \le i \le d_t} \|y_i^* - \bar{y}_i\| &\le 2\|x^* - \bar{x}\| \\ &\le 2(\|x^* - \hat{x}\| + \|\hat{x} - \bar{x}\|) \\ &\le 2(r_1 + \|\bar{x} - \hat{x}\|). \end{aligned}$$

The interpolatory cubature rule

$$E_t(f) = \frac{4\pi}{d_t} \sum_{j=1}^{d_t} f(\hat{y}_j)$$

associated with $\hat{Y}$ provides high-order numerical integration on the sphere. In particular, by Theorem 4.1 in [20], the worst-case error in a particular Sobolev space is

$$\left| \int_{S^2} f(y) d(y) - E_t(f) \right| = 4\pi D(\hat{Y}) =: e(E_t),$$

where $D(\hat{Y})$ is the Cui–Freeden generalized discrepancy [4]

$$D(\hat{Y}) = \frac{1}{2\sqrt{\pi} d_t} \left[\sum_{j=1}^{d_t} \sum_{i=1}^{d_t} \left(1 - 2\log\left(1 + \sqrt{(1 - \hat{y}_i^T \hat{y}_j)/2} \right) \right) \right]^{1/2}.$$

Table 2 gives the values $D(\hat{Y})$ and $e(E_t)$. These values are better than the values reported by Sloan and Womersley [20]. The values given in [20] use extremal points and are better than the values reported by Cui and Freeden [4].

The computed spherical t-designs with $(t+1)^2$ points are available from http://www.st.hirosaki-u.ac.jp/~chen/index.html. Computations for these low degrees were

TABLE 2
Worst case for the equal weight rule E_t and generalized discrepancy for computed spherical designs.

t	d_t	$e(E_t)$	$D(\hat{Y})$
2	9	0.349478	0.027811
3	16	0.229009	0.018239
4	25	0.162440	0.012927
5	36	0.123579	0.009834
6	49	0.098188	0.007814
7	64	0.079817	0.006352
8	81	0.067223	0.005349
9	100	0.058809	0.004680
10	121	0.049576	0.003945

performed by using MATLAB 6.1 on an IBM PC with 128MB memory and 500 MHz [15, 18].

Remark 4.1. This paper presents a new verification method for underdetermined systems of equations and uses this method to verify computed spherical t-designs. In comparison the Krawczyk-type interval operator method (1.3) failed for these underdetermined equations. This can be explained as follows.

Consider $\mathcal{K}(X)$ on an interval X which has an interior point $\hat{x}$. For any $x \in X$, $c'(x)$ is singular, and there is an x_b on the boundary of X such that $c'(x)(x_b - \hat{x}) = 0$. This implies that

$$x_b - c'(\hat{x})^+ c(\hat{x}) = \hat{x} - c'(\hat{x})^+ c(\hat{x}) + (I - c'(\hat{x})^+ c'(x))(x_b - \hat{x}) \in \mathcal{K}(X).$$

It is almost impossible to have $x_b - c'(\hat{x})^+ c(\hat{x}) \in X$ for all such boundary points x_b of X with $c'(\hat{x})^+ c(\hat{x}) \neq 0$. Hence $\mathcal{K}(X) \subseteq X$ always fails. On the other hand, the new verification method has no problems with the null space of $c'(x)$. The following example shows the advantage of the new method. Let

$$c(x) = 1 + x_1 + x_2 + x_1 x_2, \quad X = \frac{1}{4}\begin{pmatrix} [-5, -1] \\ [1+h, 3-h] \end{pmatrix}, \quad \hat{x} = \frac{1}{4}\begin{pmatrix} -3 \\ 2 \end{pmatrix},$$

where $h \in [0, 1]$. Let $\mathcal{B} = \{1\}$ and $\mathcal{N} = \{2\}$. Straightforward calculation gives

$$c(\hat{x}) = \frac{3}{8}, \quad c'(x) = (1 + x_2, 1 + x_1), \quad c'(\hat{x}) = \frac{1}{4}(6, 1), \quad c'_{\mathcal{B}}(\hat{x})^{-1} c(\hat{x}) = \frac{1}{4}.$$

It is easy to show that a Lipschitz constant for $c'_{\mathcal{B}}(x)$ is $K = 1$, and that

$$\max_{x \in N} \|c'_{\mathcal{N}}(x)\| = \frac{3}{4}.$$

Hence statement (1) of Theorem 2.1 holds with

$$\|c'_{\mathcal{B}}(\hat{x})^{-1} c(\hat{x})\| + \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \left(\frac{1}{2} K(r_1 + r_2) r_1 + \max_{x \in N} \|c'_{\mathcal{N}}(x)\| r_2\right) = \frac{1}{2} - \frac{h}{6} \le r_1 = \frac{1}{2}$$

for all $h \in [0, 1]$. Now we show that $\mathcal{K}(X) \subseteq X$ fails for all $h \in [0, 1]$. Interval calculation gives

$$c'(\hat{x})^+ C'(X) = \frac{4}{37}\begin{pmatrix} 6 \\ 1 \end{pmatrix}\left(1 + \frac{1}{4}[1+h, 3-h],\ 1 + \frac{1}{4}[-5, -1]\right),$$

$$(I - c'(\hat{x})^+ C'(X))(X - \hat{x}) = \frac{1}{37 \times 4} \begin{pmatrix} [-80 + 30h,\, 80 - 30h] \\ [-52 + 40h,\, 52 - 40h] \end{pmatrix},$$

and the radii of X and $\mathcal{K}(X)$ satisfy

$$R(X) - R(\mathcal{K}(X)) = \frac{1}{4} \begin{pmatrix} 2 \\ 1 - h \end{pmatrix} - \frac{1}{148} \begin{pmatrix} 80 - 30h \\ 52 - 40h \end{pmatrix} = \frac{1}{148} \begin{pmatrix} -6 + 30h \\ -15 + 3h \end{pmatrix}.$$

Since the second component of the radii $R_2(X) - R_2(\mathcal{K}(X)) < 0$ for all $h \in [0, 1]$, we find that $\mathcal{K}(X) \not\subseteq X$ for all $h \in [0, 1]$.

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